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RPPR Final Report

as of 12-Oct-2021

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INVESTIGATOR(S):

Name: J. Ardie Dillen
Email: Dillen@mrs.org
Phone Number: 7247792711
Principal: Y

Organization: **Materials Research Society**

Address: 506 Keystone Dr., Warrendale, PA 150867573

Country: USA

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Final Report for Period Beginning 13-Apr-2021 and Ending 31-Oct-2021

Title: 2021 Materials Research Society Spring Meeting

Begin Performance Period: 13-Apr-2021

End Performance Period: 31-Oct-2021

Report Term: 0-Other

Submitted By: Sandra Forrest

Email: forrest@mrs.org

Phone: (724) 779-2712

Distribution Statement: 1-Approved for public release; distribution is unlimited.

STEM Degrees: 0

STEM Participants:

Major Goals: Funding was requested from the Army Research Office to allow symposium organizers to cover registration fees and provide partial travel reimbursement for invited speakers, early-career researchers and students based on merit and need.

Multidisciplinary research is touted as essential to innovation. That is why, from April 17 -23, 2021, researchers working in seemingly unrelated fields gathered Virtually, to promote, share and discuss issues and developments across disciplines. The 2021 MRS Spring Meeting & Exhibit was the key forum to present research to an interdisciplinary and international audience. It provided a window on the future of materials science, and offered an opportunity for researchers—from students and postdoctoral fellows, to Nobel and Kavli Prize Laureates—to exchange technical information and network with colleagues.

Accomplishments: Symposium CT05 aligns with numerous ARL core technical competencies in Materials and Manufacturing Sciences and Computational Sciences, and included presentations by world leading researchers developing data science, machine learning and computational methods of interest to the Engineering Sciences Directorate, Materials Science Division, Information Science Directorate, and Mathematical Science Division.

Symposium EL02 - The primary goal of this symposium is to bring together world-leading experts from the academy as well as industry to exchange and share their experiences and research results on all aspects of metal-halide semiconductors for optoelectronics. This symposium will focus on a wide range of metal halide semiconductors including lead-based halide emitters, low-dimensional halide semiconductors, and non-toxic heavy-metal-free halide semiconductors to explore the fundamentals of those halide materials, including theoretical calculation, crystal/defect chemistry, carrier dynamics, photophysics, and ion migration. This symposium will also cover their use in various optoelectronic devices including light-emitting diodes, visible and infrared photodetectors, radioactive detectors, and lasers. Therefore, we believe that this symposium will promote to further advance a field of metal-halide materials, their cost-effective processing technologies, and their innovative device applications. Exploration and investigation of novel semiconducting materials like halide semiconductors would be very beneficial for the Army Research Office (ARO)'s research areas, especially (1) Optoelectronics and (2) Electronic sensing, including semiconductor lasers and optical sensors in the UV/visible/infrared spectral ranges.

Symposium EL03 - A symposium focused on complex-structured semiconductors was a valuable addition to the MRS Spring Meeting. The research communities interested in complex chalcogenide and nitride semiconductors are growing rapidly. The MRS has in the past featured symposia on physical properties of complex oxides, but this rich field has been somewhat underrepresented at recent Spring and Fall meetings. The symposium converge

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these communities with a unified focus on the unique opportunities and challenges presented by designing, making, and using semiconductors.

The topics and themes covered by symposium EL03 fit very well within the purview of ARO programs in Materials Science including Physical Properties of Materials, and Synthesis and Processing of Materials (cognizant program managers Dr. Pani Varanasi and Dr. Michal Bakas). Symposium EL03 is distinguished by its focus on processing-properties-performance links, with a scope extending from theory and fundamentals, to nano-structured materials, to wafer-scale film processing, and a focus throughout on what applications can be uniquely enabled by the properties of ionic semiconductors. This connection from physics and chemistry, to materials science, to electrical and application engineering is shared by the ARO and is important to developing complex-structured and multicomponent material systems into solutions for the Army.

Applications and enabling methods covered by EL03 and relevant to ARO include:

- High-speed and low-power photonics for computing and communications
- Reconfigurable optics
- Analog and neuromorphic computing implemented using memristors and phase-change materials
- Wafer-scale growth of single-crystal, epitaxial 2D materials
- Lightweight and durable photovoltaics
- Directed synthesis of nano-structured semiconductor composites

Symposium SM12 - This symposium covered recent advances in the development of bioinspired materials. The following topics were included into this symposium: (1) Biomimetic formation of inorganic (nano)crystals (e.g. composite crystals, metal oxides and plasmonic nanoparticles); (2) Biomineralization; (3) In situ characterization of bio-inspired assembly and bio-controlled crystal formation; (4) Theory driven design of (bio)macromolecules for self-assembly and for controlling inorganic crystal formation; (5) Hierarchical assembly of proteins, peptides, DNAs, peptoids and biomimetic polymers into nanostructured materials, including biomimetic membranes, nanotubes and hydrogels. This symposium, highlighted recent developments in exploiting (bio)macromolecules 1) for self-assembly of soft matter with hierarchical structures, and 2) for controlling inorganic (nano)crystal nucleation and growth and assembly of inorganic (nano)crystals into superstructures. It addressed 3) the most recent insights obtained in the principles underlying (bio)macromolecular self-assembly, bio-controlled crystal formation and biomineralization (including using in situ molecular imaging and computational tools).

Training Opportunities: Nothing to Report

Results Dissemination: The program for the MRS 2021 Virtual Spring meeting is posted to our website: www.mrs.org

Honors and Awards: Nothing to Report

Protocol Activity Status:

Technology Transfer: Nothing to Report

PARTICIPANTS:

Participant Type: Other Professional

Participant: Ki Tae Nam

Person Months Worked: 1.00

Project Contribution:

National Academy Member: N

Funding Support:

Participant Type: Other Professional

Participant: Fiona Meldrum

Person Months Worked: 1.00

Project Contribution:

National Academy Member: N

Funding Support:

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as of 12-Oct-2021

Partners

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I certify that the information in the report is complete and accurate:

Signature: Sandra Forrest

Signature Date: 10/11/21 10:50AM

FINAL REPORT – S21 Symposium CT05, Artificial Intelligence and Automation for Materials Design

Amanda Barnard, Australian National University

Krishna Rajan, University of New York at Buffalo

Bronwyn Fox, Swinburne University of Technology

Ibo Mathews, Lawrence Livermore National Laboratory

Objectives

The objectives for S21 Symposium CT05, Artificial Intelligence and Automation for Materials Design, were to demonstrate best practice in materials informatics, by showcasing presentations from leading researchers from round the world. The symposium captured a diversity of materials and materials challenges, and explored the use of a range of different machine learning and automation approaches, rather than focusing on one class of materials or methods.

Presentations

S21 Symposium CT05, Artificial Intelligence and Automation for Materials Design, hosted 18 invited speakers, 59 contributed oral presentations and 10 poster presentations. The final program is attached in Appendix A. These presentations were group in 6 different topic areas involving the use of similar methods, data sets or instruments, but covering multiple different materials. These topics were Machine Learning (2 sessions), Materials Informatics (2 sessions), Applications (3 sessions) Automation of High Throughput (2 sessions) Data-driven Chemistry (3 sessions), and Deep Learning and Computer Vision (1 session). All session were well attended, as the timing of each session in a give group was scheduled for either morning, afternoon or evening, to allow geographically diverse participation across all topic areas.

Highlights

Highlights of Symposium S21 Symposium CT05, Artificial Intelligence and Automation for Materials Design, include the world leading invited speaker that attracted a large audience, particularly Prof Chris Wolverton, Prof. Krishna Rajan, Dr Anuhav and Prof Nicola Mazari. The Symposium also offered a tutorial on the use of the AFLOW materials informatics platform by the team of invited speaker Prof Stefano Curtarolo.

Contributions to Discipline

Symposium S21 Symposium CT05, Artificial Intelligence and Automation for Materials Design, has among the first in the materials community to present cutting edge research using graph machine learning, adversarial learning and coupling of deep learning and computer vision with micronanalysis instrumentation such as electron microscopy, scanning probe microscopy and atom probe tomography.

Future Direction for this Symposium

As the materials community become more familiar with machine learning, artificial intelligence and cyberphysical systems, the opportunity to continue and expand this symposium will grow. The value of the Symposium is not in providing an annual repetition of established methods applied to a new set of materials, but rather it is the demonstration of new set of cutting-edge methods that can address emerging materials challenges that cannot be solved using existing technology. For example, as new machine learning methods are developed in computer science, the opportunity to introduce new sessions demonstrating their efficacy in materials discovery and design. This mean the Symposium will always be disruptive, rather than presenting iterative advances and eventually reaching a steady state.

APPENDIX A

Session Information							
SESSION TITLE: CT05.01: Machine Learning I							
SESSION TYPE: Oral							
SESSION DAY & DATE: Sun 4/18/2021 8:00 AM							
SESSION DURATION: 105							
SESSION LOCATION: CT05							
SESSION HOST: Session Chair: Krishna Rajan Session Chair: Thomas Hammerschmidt							
SESSION TOPIC: CT05: Artificial Intelligence and Automation for Materials Design							
SESSION ABBREVIATION: CT05.01							
Control ID	Final ID	Title	Presenting Author	Presentation Type	Start/end time	PRESENTER (COUNTRY ONLY)	SESSION ABSTRACT DURATION
<u>3502694</u>	CT05.01.01	Network Theory Meets Materials Science	Wolverton, Christopher	Invited Speaker	8:00 AM 8:25 AM	United States	25
<u>3563912</u>	CT05.01.02	Late News: Optimizing Complex Geometries with Feed Forward Control and Machine Learning	Druzgalski, Clara	Oral Presentation Preferred	8:25 AM 8:40 AM	United States	15
<u>3491835</u>	CT05.01.03	Natural Language Processing for Materials Design—What Can We Extract From the Research Literature?	Jain, Anubhav	Invited Speaker	8:40 AM 9:05 AM	United States	25
<u>3498621</u>	CT05.01.04	Natural Language Processing for Insensitivity Classification of Energetic Materials	Kumar, Gaurav	Oral Presentation Preferred	9:05 AM 9:20 AM	United States	15
<u>3501386</u>	CT05.01.05	Active Materials Exploration and Characterization with Bayesian Optimization	Rinke, Patrick	Invited Speaker	9:20 AM 9:45 AM	Finland	25

Session Information							
SESSION TITLE: CT05.02: Automation and High Throughput I							
SESSION TYPE: Oral							
SESSION DAY & DATE: Sun 4/18/2021 10:30 AM							
SESSION DURATION: 90							
SESSION LOCATION: CT05							
SESSION HOST: Session Chair: Prahalada Rao Session Chair: Nicholas Kotov							
SESSION TOPIC: CT05: Artificial Intelligence and Automation for Materials Design							
SESSION ABBREVIATION: CT05.02							
Control ID	Final ID	Title	Presenting Author	Presentation Type	Start/end time	PRESENTER (COUNTRY ONLY)	SESSION ABSTRACT DURATION
3502635	CT05.02.01	Materials Informatics and Manufacturing Scalability and Sustainability	Olivetti, Elsa	Invited Speaker	10:30 AM 10:55 AM	United States	25
3515420	CT05.02.02	Automated Multimodal Manufacturing Optimization	Giera, Brian	Invited Speaker	10:55 AM 11:20 AM	United States	25
3498429	CT05.02.03	Autonomous End-to-End Systems for Materials Discovery	Aykol, Muratahan	Invited Speaker	11:20 AM 11:45 AM	United States	25
3487822	CT05.02.04	Robotics-Enabled Exploration of Multicomponent Lead Halide Perovskites via Machine Learning	Higgins, Kate	No Preference	11:45 AM 12:00 PM	United States	15

Session Information							
SESSION TITLE: CT05.03: Applications I							
SESSION TYPE: Oral							
SESSION DAY & DATE: Sun 4/18/2021 1:00 PM							
SESSION DURATION: 95							
SESSION LOCATION: CT05							
SESSION HOST: Session Chair: Sanket Deshmukh Session Chair: Steven Torrisi							
SESSION TOPIC: CT05: Artificial Intelligence and Automation for Materials Design							
SESSION ABBREVIATION: CT05.03							
Control ID	Final ID	Title	Presenting Author	Presentation Type	Start/end time	PRESENTER (COUNTRY ONLY)	SESSION ABSTRACT DURATION
3502595	CT05.03.01	Machine Learning for the Modeling of Complex Energy Materials	Artrith, Nongnuch	Invited Speaker	1:00 PM 1:25 PM	United States	25
3495315	CT05.03.02	Automated <i>In Silico</i> Screening of Nanoporous Materials for Enhanced CO ₂ Capture	Neumann, Rodrigo	Oral Presentation Preferred	1:25 PM 1:40 PM	Brazil	15
3563026	CT05.03.03	Late News: Machine Learning with Persistent Homology and Chemical Word Embeddings Improves Predictive Accuracy and Interpretability in Metal-Organic Frameworks	Montoya, Joseph	Oral Presentation Preferred	1:40 PM 1:55 PM	United States	15
3502238	CT05.03.04	Defect Detection and Uncertainty Quantification in Property Prediction with Machine Learning	Morgan, Dane	Invited Speaker	1:55 PM 2:20 PM	United States	25
3483721	CT05.03.05	Machine Learning the Quantum-Chemical Properties of Metal-Organic Frameworks for Accelerated Materials Discovery with a New Electronic Structure Database	Rosen, Andrew	Oral Presentation Preferred	2:20 PM 2:35 PM	United States	15

Session Information							
SESSION TITLE: CT05.04: Material Informatics I							
SESSION TYPE: Oral							
SESSION DAY & DATE: Sun 4/18/2021 4:00 PM							
SESSION DURATION: 100							
SESSION LOCATION: CT05							
SESSION HOST: Session Chair: Mathieu Bauchy Session Chair: Wujie Wang							
SESSION TOPIC: CT05: Artificial Intelligence and Automation for Materials Design							
SESSION ABBREVIATION: CT05.04							
Control ID	Final ID	Title	Presenting Author	Presentation Type	Start/end time	PRESENTER (COUNTRY ONLY)	SESSION ABSTRACT DURATION
3490040	CT05.04.01	Understanding and Visualizing Hyperspectral ToF-SIMS Data Sets Using Machine Learning	Pigram, Paul	Invited Speaker	4:00 PM 4:25 PM	Australia	25
3491637	CT05.04.02	Charting the Low-Loss Region in Electron Energy Loss Spectroscopy with Machine Learning	Rojo, Juan	Oral Presentation Preferred	4:25 PM 4:40 PM	Netherlands	15
3501102	CT05.04.03	Discovery of Interpretable X-Ray Absorption Spectroscopy Signatures via Random Forest Machine Learning Models	Torrissi, Steven	Oral Presentation Preferred	4:40 PM 4:55 PM	United States	15
3563854	CT05.04.04	Late News: Machine Learning Force Fields for Understanding the Thermodynamics of Li-Ion Cathodes	Gabriel, Joshua	No preference	4:55 PM 5:00 PM	United States	5
3496730	CT05.04.05	Improvement of Adhesion Between NiTi Alloy and Diamond-Like Carbon Film by Bayesian Optimization	Toyonaga, Masafumi	Poster Presentation Preferred	5:00 PM 5:05 PM	Japan	5
3501986	CT05.04.06	High-Throughput Electrochemical Screening of Deep Eutectic Solvent for Use in Redox Flow Batteries	Politi, Maria	Poster Presentation Preferred	5:05 PM 5:10 PM	United States	5
3560296	CT05.04.07	Late News: A Materials-Informatics Based Study of Solid Electrolytes and Protective Coatings for Li Batteries	Honrao, Shreyas	Oral Presentation Preferred	5:10 PM 5:25 PM	United States	15
3559364	CT05.04.08	Late News: Prediction of Bulk and Grain Boundary Ionic Conductivities for Solid-State Li-Ion Conductors by Machine Learning	Wu, Yen-Ju	Oral Presentation Preferred	5:25 PM 5:40 PM	Japan	15

Session Information							
SESSION TITLE: CT05.05: Machine Learning II							
SESSION TYPE: Oral							
SESSION DAY & DATE: Sun 4/18/2021 6:30 PM							
SESSION DURATION: 85							
SESSION LOCATION: CT05							
Session Chair: Krishna Rajan							
SESSION HOST: Session Chair: Rodrigo Neumann							
Session Chair: Clara Druzgalski							
SESSION TOPIC: CT05: Artificial Intelligence and Automation for Materials Design							
SESSION ABBREVIATION: CT05.05							
Control ID	Final ID	Title	Presenting Author	Presentation Type	Start/end time	PRESENTER (COUNTRY ONLY)	SESSION ABSTRACT DURATION
3498999	CT05.05.01	End-to-End Differentiability and Tensor Processing Unit Computing to Accelerate Materials' Inverse Design	Bauchy, Mathieu	Invited Speaker	6:30 PM 6:55 PM	United States	25
3501865	CT05.05.02	Solving Inverse Problems with Differentiable Molecular Dynamics	Wang, Wujie	Oral Presentation Preferred	6:55 PM 7:10 PM	United States	15
3500723	CT05.05.03	Graphical Model Parameters for Formation of 3D Nanomolecular Complexes	Cha, Minjeong	Oral Presentation Preferred	7:10 PM 7:25 PM	United States	15
3516240	CT05.05.04	Graph Theory for Design of Complex Biomimetic Nanostructures	Kotov, Nicholas	Oral Presentation Preferred	7:25 PM 7:40 PM	United States	15
3501051	CT05.05.05	Symmetry Incorporated Graph Convolutional Neural Networks for Solid-State Materials	Gong, Weiyi	Oral Presentation Preferred	7:40 PM 7:55 PM	United States	15

Session Information							
SESSION TITLE: CT05.06: Materials Informatics II							
SESSION TYPE: Oral							
SESSION DAY & DATE: Mon 4/19/2021 8:00 AM							
SESSION DURATION: 110							
SESSION LOCATION: CT05							
SESSION HOST: Session Chair: Stefano Curtarolo Session Chair: Nuwan Dewapriya							
SESSION TOPIC: CT05: Artificial Intelligence and Automation for Materials Design							
SESSION ABBREVIATION: CT05.06							
Control ID	Final ID	Title	Presenting Author	Presentation Type	Start/end time	PRESENTER (COUNTRY ONLY)	SESSION ABSTRACT DURATION
<u>3516946</u>	CT05.06.01	Artificial Intelligence Towards Materials Maps	Scheffler, Matthias	Invited Speaker	8:00 AM 8:25 AM	Germany	25
<u>3501478</u>	CT05.06.02	The Search for New Materials	Pitfield, Joe	Oral Presentation Preferred	8:25 AM 8:40 AM	United Kingdom	15
		Break			8:40 AM 8:55 AM		15
<u>3501996</u>	CT05.06.04	Digital Infrastructures for Materials Research and Discovery	Marzari, Nicola	Invited Speaker	8:55 AM 9:20 AM	Switzerland	25
<u>3502496</u>	CT05.06.05	Automated Microstructural Feature Extraction for Accelerated Materials Discovery	Wodo, Olga	Oral Presentation Preferred	9:20 AM 9:35 AM	United States	15
<u>3502765</u>	CT05.06.06	MPDD: Material-Property-Descriptor Database	Krajewski, Adam	Oral Presentation Preferred	9:35 AM 9:50 AM	United States	15

Session Information							
SESSION TITLE: CT05.07: Data-Driven Chemistry I							
SESSION TYPE: Oral							
SESSION DAY & DATE: Mon 4/19/2021 10:30 AM							
SESSION DURATION: 50							
SESSION LOCATION: CT05							
SESSION HOST: Session Chair: Casey Brock							
SESSION TOPIC: CT05: Artificial Intelligence and Automation for Materials Design							
SESSION ABBREVIATION: CT05.07							
Control ID	Final ID	Title	Presenting Author	Presentation Type	Start/end time	PRESENTER (COUNTRY ONLY)	SESSION ABSTRACT DURATION
<u>3502279</u>	CT05.07.01	Inverse Design of Self-Reporting Redox-Active Materials Using Quantum Chemistry Guided Active Learning	Agarwal, Garvit	Oral Presentation Preferred	10:30 AM 10:45 AM	United States	15
<u>3501950</u>	CT05.07.02	Accelerated Prediction of Atomically Precise Cluster Structures Using On-the-Fly Active Learning	Wang, Yunzhe	Oral Presentation Preferred	10:45 AM 11:00 AM	United States	15
<u>3502024</u>	CT05.07.03	Screening and Understanding Li Adsorption on Two-Dimensional Metallic Materials by Learning Physics	Gong, Sheng	Oral Presentation Preferred	11:00 AM 11:15 AM	United States	15
<u>3502533</u>	CT05.07.04	Multi-Fidelity Information Fusion DFT Study of Doped-Graphene Single Atom Catalysts	Wahab, Hud	Poster Presentation Preferred	11:15 AM 11:20 AM	United States	5

Session Information							
SESSION TITLE: CT05.08: Applications II							
SESSION TYPE: Oral							
SESSION DAY & DATE: Mon 4/19/2021 1:00 PM							
SESSION DURATION: 110							
SESSION LOCATION: CT05							
SESSION HOST: Session Chair: Patrick Parkinson Session Chair: Andrew Rosen							
SESSION TOPIC: CT05: Artificial Intelligence and Automation for Materials Design							
SESSION ABBREVIATION: CT05.08							
Control ID	Final ID	Title	Presenting Author	Presentation Type	Start/end time	PRESENTER (COUNTRY ONLY)	SESSION ABSTRACT DURATION
3519293	CT05.08.01	Investigating the Shapes of Bottlebrush Polymers Using Machine Learning	Deshmukh, Sanket	Invited Speaker	1:00 PM 1:25 PM	United States	25
3516234	CT05.08.02	Searching Order within Disorder with AI-Automation	Curtarolo, Stefano	Invited Speaker	1:25 PM 1:50 PM	United States	25
3499131	CT05.08.03	A Phase Mapping Algorithm to Accelerate High Throughput Experiments	Chang, Ming-Chiang	Oral Presentation Preferred	1:50 PM 2:05 PM	United States	15
3499748	CT05.08.04	High Dimensional Model Representation - Gaussian Process Regression—A Powerful Tool to Learn Multivariate Functions from Sparse Data	Manzhos, Sergei	Oral Presentation Preferred	2:05 PM 2:20 PM	Canada	15
3501852	CT05.08.05	Comprehensive Comparison of Modern Sequential Design Approaches for Material Optimization—Application to Metal-Organic Frameworks	Trezza, Giovanni	Oral Presentation Preferred	2:20 PM 2:35 PM	Italy	15
3502781	CT05.08.06	Machine Learning Tools to Accelerate Scalable Perovskite PV Manufacturing	Rolston, Nicholas	Oral Presentation Preferred	2:35 PM 2:50 PM	United States	15

Session Information							
SESSION TITLE: CT05.09: Materials Informatics III							
SESSION TYPE: Oral							
SESSION DAY & DATE: Mon 4/19/2021 4:00 PM							
SESSION DURATION: 120							
SESSION LOCATION: CT05							
SESSION HOST: Session Chair: Muratahan Aykol Session Chair: Bin Ouyang							
SESSION TOPIC: CT05: Artificial Intelligence and Automation for Materials Design							
SESSION ABBREVIATION: CT05.09							
Control ID	Final ID	Title	Presenting Author	Presentation Type	Start/end time	PRESENTER (COUNTRY ONLY)	SESSION ABSTRACT DURATION
3502358	CT05.09.01	Towards Small-Data-Driven Materials Science	Ghiringhelli, Luca	Invited Speaker	4:00 PM 4:25 PM	Germany	25
3498765	CT05.09.02	Data-Driven Quantum Dot Synthesis Development in Flow	Abolhasani, Milad	Oral Presentation Preferred	4:25 PM 4:40 PM	United States	15
3500977	CT05.09.03	Machine Learning Prediction of Creep Rupture Behavior for Metal Alloys	Jamshidi, Reihaneh	No Preference	4:40 PM 4:45 PM	United States	5
3497846	CT05.09.04	Development of an Artificial Intelligence (AI) Based Image Processing Tool to Detect Microstructural Variations in AM Ti-6Al-4V	Casukhela, Rohan	Poster Presentation Preferred	4:45 PM 4:50 PM	United States	5
3501649	CT05.09.05	Coupling Machine Learning and Physics-Based Simulations to Accelerate Materials Design	Meredig, Bryce	Invited Speaker	4:50 PM 5:15 PM	United States	25
3495027	CT05.09.06	Predicting Fracture Stress of Defective Graphene Samples Using Artificial Neural Networks	Dewapriya, Nuwan	Oral Presentation Preferred	5:15 PM 5:30 PM	Canada	15
3502158	CT05.09.07	Explaining Neural Network Predictions of Material Strength	Mundhenk, Terrell	Oral Presentation Preferred	5:30 PM 5:45 PM	United States	15

Session Information							
SESSION TITLE: CT05.10: Deep Learning and Computer Vision							
SESSION TYPE: Oral							
SESSION DAY & DATE: Mon 4/19/2021 8:10 PM							
SESSION DURATION: 125							
SESSION LOCATION: CT05							
SESSION HOST: Session Chair: Paul Pigram Session Chair: Olga Wodo							
SESSION TOPIC: CT05: Artificial Intelligence and Automation for Materials Design							
SESSION ABBREVIATION: CT05.10							
Control ID	Final ID	Title	Presenting Author	Presentation Type	Start/end time	PRESENTER (COUNTRY ONLY)	SESSION ABSTRACT DURATION
3501902	CT05.10.02	Using Deep Learning to Find High Performance Phase-Change Switchable Metasurface Reflectors	Thompson, Jonathan	Oral Presentation Preferred	8:10 PM 8:25 PM	United States	15
3562922	CT05.10.03	Late News: Automatic Characterization of Single-Walled Carbon Nanotube Film Morphologies Using Computer Vision	Williams, Phillip	Oral Presentation Preferred	8:25 PM 8:40 PM	Canada	15
3483923	CT05.10.04	Image Deconvolution and Resolution Enhancement in Scanning Probe Microscopy Using Deep Learning	Bonagiri, Lalith Krishna Samanth	Oral Presentation Preferred	8:40 PM 8:55 PM	United States	15
		Break			8:55 PM 9:10 PM		15
3494302	CT05.10.05	Rapid and Flexible Classification of Scanning Transmission Electron Microscopy Data Using Few Shot Learning	Akers, Sarah	Oral Presentation Preferred	9:10 PM 9:25 PM	United States	15
3500915	CT05.10.06	Machine Learning to Reveal Nanoparticle Dynamics from Liquid-Phase TEM Videos	Yao, Lehan	No Preference	9:25 PM 9:30 PM	United States	5
3500684	CT05.10.07	Deep Learning for Super-Resolved Atomistic Predictions from Atom Probe Tomography	Sonal, Aditi	Oral Presentation Preferred	9:30 PM 9:45 PM	United States	15
3537837	CT05.10.08	Late News: Advances in Image Driven Machine Learning for Microstructure Recognition and Characterization	Baskaran, Arun	Oral Presentation Preferred	9:45 PM 10:00 PM	United States	15
3502054	CT05.10.09	Leveraging Uncertainty from Deep Learning for Trustworthy Materials Discovery Workflows	Zhang, Jize	Oral Presentation Preferred	10:00 PM 10:15 PM	United States	15

Session Information							
SESSION TITLE: CT05.11: Applications III							
SESSION TYPE: Oral							
SESSION DAY & DATE: Tue 4/20/2021 8:00 AM							
SESSION DURATION: 110							
SESSION LOCATION: CT05							
SESSION HOST: Session Chair: Dane Morgan Session Chair: Manyalibo Matthews							
SESSION TOPIC: CT05: Artificial Intelligence and Automation for Materials Design							
SESSION ABBREVIATION: CT05.11							
Control ID	Final ID	Title	Presenting Author	Presentation Type	Start/end time	PRESENTER (COUNTRY ONLY)	SESSION ABSTRACT DURATION
3516228	CT05.11.01	Machine Learning Aided Discovery of Patterns in Crystal Chemistry	Rajan, Krishna	Invited Speaker	8:00 AM 8:25 AM	United States	25
3501711	CT05.11.02	Discovering Relationships Between OSDAs and Zeolites Through Data Mining and Generative Neural Networks	Jensen, Zachary	Oral Presentation Preferred	8:25 AM 8:40 AM	United States	15
3502077	CT05.11.03	Graph-Based Deep Learning for Designing Stable Interfaces for Solid-State Batteries	Pandey, Shubham	Oral Presentation Preferred	8:40 AM 8:55 AM	United States	15
3505443	CT05.11.04	Machine Learning Stability Rules for Complex Ionic Compounds and Its Application in the Discovery of New NASICON Materials	Ouyang, Bin	Oral Presentation Preferred	8:55 AM 9:10 AM	United States	15
3501767	CT05.11.05	Combining Machine Learning and Multiscale Modeling for Accelerated Battery Manufacturing Optimization	Franco, Alejandro	Invited Speaker	9:10 AM 9:35 AM	France	25
3501492	CT05.11.06	Calibration of Thermal Spray Microstructure Simulations to Experimental Data Using Bayesian Optimization	Montes de Oca Zapiain, David	Oral Presentation Preferred	9:35 AM 9:50 AM	United States	15

Session Information							
SESSION TITLE: CT05.12: Data-Driven Chemistry II							
SESSION TYPE: Oral							
SESSION DAY & DATE: Tue 4/20/2021 11:45 AM							
SESSION DURATION: 85							
SESSION LOCATION: CT05							
SESSION HOST: Session Chair: Alejandro Franco Session Chair: Shubham Pandey							
SESSION TOPIC: CT05: Artificial Intelligence and Automation for Materials Design							
SESSION ABBREVIATION: CT05.12							
Control ID	Final ID	Title	Presenting Author	Presentation Type	Start/end time	PRESENTER (COUNTRY ONLY)	SESSION ABSTRACT DURATION
3501486	CT05.12.01	Machine-Learning the Structural Stability of Intermetallic Phases with Domain Knowledge of the Interatomic Bond	Hammerschmidt, Thomas	Invited Speaker	11:45 AM 12:10 PM	Germany	25
3563139	CT05.12.02	Late News: Machine Learning Potentials for Copper Alloys	Diaz Carral, Angel	Oral Presentation Preferred	12:10 PM 12:25 PM	Germany	15
3561183	CT05.12.03	Late News: Investigating Representations of Local Atomic Environments with Topology Optimization	Debnath, Arindam	Oral Presentation Preferred	12:25 PM 12:40 PM	United States	15
3563809	CT05.12.04	Late News: Machine Learning Prediction of the Hubbard U for Materials Containing Transition Metals	Brock, Casey	Oral Presentation Preferred	12:40 PM 12:55 PM	United States	15
3502296	CT05.12.05	Automated Training of Many-Body Machine Learned Force Fields	Vandermause, Jonathan	Oral Presentation Preferred	12:55 PM 1:10 PM	United States	15

Session Information							
SESSION TITLE: CT05.13: Automation and High Throughput II							
SESSION TYPE: Oral							
SESSION DAY & DATE: Tue 4/20/2021 2:15 PM							
SESSION DURATION: 115							
SESSION LOCATION: CT05							
SESSION HOST: Session Chair: Brian Giera Session Chair: Kate Higgins							
SESSION TOPIC: CT05: Artificial Intelligence and Automation for Materials Design							
SESSION ABBREVIATION: CT05.13							
Control ID	Final ID	Title	Presenting Author	Presentation Type	Start/end time	PRESENTER (COUNTRY ONLY)	SESSION ABSTRACT DURATION
3515415	CT05.13.01	Heterogeneous Sensing and Scientific Machine Learning for Quality Assurance in Laser Powder Bed Fusion	Rao, Prahalada	Invited Speaker	2:15 PM 2:40 PM	United States	25
3484435	CT05.13.02	High-Throughput Correlative Microscopy and Spectroscopy for Nano-Laser Development	Parkinson, Patrick	Oral Presentation Preferred	2:40 PM 2:55 PM	United Kingdom	15
3502102	CT05.13.03	Implementation of Benchtop NMR as an Online, High-Throughput Sensor in Automated Synthesis Systems	Le-McClain, Anh	Oral Presentation Preferred	2:55 PM 3:10 PM	United States	15
3502136	CT05.13.04	High-Throughput and Data-Driven Strategies for the Design of Deep Eutectic Solvent Electrolytes	Rodriguez, Jaime	Oral Presentation Preferred	3:10 PM 3:25 PM	United States	15
3502313	CT05.13.05	Machine Learning Modeling of Photodiode Signal for Selection of Laser Parameters in Laser Powder Bed Fusion Additive Manufacturing	Lapointe, Simon	Oral Presentation Preferred	3:25 PM 3:40 PM	United States	15
3502888	CT05.13.06	Decision Trees in Continuous Action Space for High-Throughput Exploration of Potential Energy Surface of Nanoclusters	Manna, Sukriti	Oral Presentation Preferred	3:40 PM 3:55 PM	United States	15
3562241	CT05.13.07	Late News: High-Throughput Reaction Screening for Accelerated Materials Research	Mustard, Thomas	Oral Presentation Preferred	3:55 PM 4:10 PM	United States	15

Session Information							
SESSION TITLE: CT05.14: Data-Driven Chemistry III							
SESSION TYPE: Oral							
SESSION DAY & DATE: Tue 4/20/2021 9:25 PM							
SESSION DURATION: 45							
SESSION LOCATION: CT05							
SESSION HOST: Session Chair: Yen-Ju Wu Session Chair: Sukriti Manna							
SESSION TOPIC: CT05: Artificial Intelligence and Automation for Materials Design							
SESSION ABBREVIATION: CT05.14							
Control ID	Final ID	Title	Presenting Author	Presentation Type	Start/end time	PRESENTER (COUNTRY ONLY)	SESSION ABSTRACT DURATION
3502548	CT05.14.02	Unique Challenges on NNP Development and Ways to Overcome Them	Jeong, Wonseok	Oral Presentation Preferred	9:25 PM 9:40 PM	Korea (the Republic of)	15
3550610	CT05.14.03	Late News: Analysis on the Strengthening Mechanism of Aluminum Alloys with Bayesian Learning for Neural Networks	Takemoto, Shimpei	Oral Presentation Preferred	9:40 PM 9:55 PM	Japan	15
3500051	CT05.14.04	Accurate Band-Gap Database for Semiconducting Inorganic Materials—Implementation of Hybrid Functional	Kim, Sangtae	Poster Presentation Preferred	9:55 PM 10:00 PM	Korea (the Republic of)	5
3500476	CT05.14.05	Developing Machine-Learning Potentials from Disordered Structures for Crystal Structure Prediction	Hong, Changho	Poster Presentation Preferred	10:00 PM 10:05 PM	Korea (the Republic of)	5
3500613	CT05.14.06	Efficient Sampling for Training Set of Machine Learning Potentials Using Metadynamics	Jung, Jisu	Poster Presentation Preferred	10:05 PM 10:10 PM	Korea (the Republic of)	5

FINAL REPORT – F21 Symposium EL02, Fundamentals of Halide Semiconductors for Optoelectronics

Do Young Kim, Oklahoma State University

Jong Hyun Kim, Ajou University

William W. Yu, Louisiana State University

Xue Bai, Jilin University

Objectives

The objectives of S21 Symposium EL02: Fundamentals of Halide Semiconductors for Optoelectronics were to bring together world-leading experts from the academy as well as industry to exchange and share their experiences and research results on all aspects of metal-halide semiconductors for optoelectronics. This symposium captured a wide range of metal halide semiconductors including lead-based halide emitters, low-dimensional halide semiconductors, and non-toxic heavy-metal-free halide semiconductors to explore the fundamentals of those halide materials, including theoretical calculation, crystal/defect chemistry, carrier dynamics, photophysics, and ion migration. This symposium also covered their use in various optoelectronic devices including light-emitting diodes, visible and infrared photodetectors, radioactive detectors, and lasers.

Presentations

S21 Symposium EL02: Fundamentals of Halide Semiconductors for Optoelectronics hosted 20 invited speakers, 48 contributed oral presentations and 4 poster presentations. The final program is attached in Appendix A. These presentations were group in 7 different topic areas involving the use of similar methods, data sets or instruments, but covering multiple different materials. These topics were Low-Dimensional Halide Semiconductors (2 sessions), Non-Toxic Heavy-Metal-Free Halide Semiconductors (1 session), Synthesis and Crystal/Defect Chemistry of Halide Semiconductors (2 sessions), Carrier Dynamics and Transportation Mechanisms (2 sessions), Photophysics of Halide Semiconductors (2 sessions) Halide Perovskite LEDs (2 sessions), and Halide-Based Detectors (1 session). All session were well attended, as the timing of each session in a given group was scheduled for either morning, afternoon or evening, to allow geographically diverse participation across all topic areas.

Highlights

Highlights of S21 Symposium EL02: Fundamentals of Halide Semiconductors for Optoelectronics include the world leading invited speaker that attracted a large audience, particularly Prof. David Mitzi, Prof. Antoine Kahn, Prof. Tae-Woo Lee, Prof. Hin-Lap Yip, Prof. Jinsong Huang, and Prof. Libai Huang.

Contributions to Discipline

S21 Symposium EL02: Fundamentals of Halide Semiconductors for Optoelectronics has provided the materials community with cutting-edge research synthesizing a variety of novel halide semiconductors, investigating their optoelectronic material properties, and applying them to unique optoelectronic device architectures.

Future Direction for this Symposium

As a new class of optoelectronic materials, S21 Symposium EL02: Fundamentals of Halide Semiconductors for Optoelectronics focused on exploring the fundamentals of a wide range of metal halide semiconductors by using theoretical calculation, crystal/defect chemistry, carrier dynamics, photophysics, and ion migration. However, applications of these novel halide semiconductors to optoelectronic devices will be more important for practical applications. Therefore, the future symposium will be expanded to cover more device researches. In addition to the fundamental researches focused on this symposium, temporal stability and large-area fabrication of the halide semiconductor films and optoelectronic devices related to production will be also included.

Final Report

Army Research Office Grant No. W911NF-21-1-0142-(78778-MS-CF)

Rafael Jaramillo, Massachusetts Institute of Technology, September 11, 2021

1. Objectives

The objective of this grant was to support participation in Symposium EL03, *Emerging Ionic Semiconductors Research and Applications*, which was part of the Materials Research Society Spring Meeting 2021. This symposium was devoted to research on semiconductor materials characterized by ionic chemical bonding, and that that are potentially of use for applications including solid state lighting, energy conversion, high-frequency telecommunications, photocatalysis, and transparent electronics.

2. Presentations

Symposium EL03 featured 44 presentations and one panel discussion. Here we list the invited presenters and their presentation titles:

- Ulrich Aschauer, University of Bern
 - Surface Structure, Defects and Reactivity of Perovskite Oxynitrides
- Megan Butala, University of Florida
 - Structure-Property Relationships in Complex Early Transition Metal Oxides for High-Rate Energy Storage
- Kazunari Domen, University of Tokyo
 - Efficient Photocatalysts for Water Splitting to Produce Solar Hydrogen
- Hideo Hosono, Tokyo Institute of Technology
 - Progress in Wide Gap Ionic Oxide Semiconductors
- Karsten Jacobsen, Technical University of Denmark
 - Computational Screening of Light-Absorbing Materials for Tandem Devices
- Mercuri Kanatzidis, Northwestern University
 - Challenges and Opportunities in Ionic Chalcogenide Semiconductors
- Joseph Bennett, University of Maryland Baltimore
 - Data-Enabled Discovery of New Semiconductors for Energy Generation and Energy Storage
- Karin Rabe, Rutgers
 - Electron Count and Ferroelectricity in Complex Oxides From First Principles
- Jayakanth Ravichandran, University of Southern California
 - Thin Film Growth of Chalcogenide Perovskites by Pulsed Laser Deposition
- David Scanlon, University College London
 - Prediction of Novel Quinary Layered Oxychalcogenides
- Kimberly See, California Institute of Technology
 - Divalent Ion Conductors
- Zhimei Sun, Beihang University

- Composition-Gradient- Mediated Semiconductor- Metal Transition in Ternary Transition-Metal-Dichalcogenide Bilayers
- Matthias Wuttig, RWTH Aachen University
 - Metavalent Bonding in Solids —Provocation or Promise?
- Andriy Zakutayev, National Renewable Energy Laboratory
 - Materials Chemistry of Ternary Nitride Semiconductors
- Alexandra Zevalkink, Michigan State University
 - Origin of Unexpectedly Low Thermal Conductivity in Mg₃Sb₂ and Mg₃Bi₂ Thermoelectric Materials

EL03 also featured a panel discussion on the theme “*Why New Semiconductors?*” with participants:

- Panelists
 - Hideo Hosono, Tokyo Institute of Technology
 - George Nolas, University of Florida
 - Andriy Zakutayev, National Renewable Energy Laboratory
 - Shengbai Zheng, Rensselaer Polytechnic University
- Moderator
 - Rafael Jaramillo, Massachusetts Institute of Technology

3. Highlights

Two presenters were recognized by Best Oral Awards from the MRS.

- Jacob Cordell, from Colorado School of Mines and National Renewable Energy Laboratory, was recognized for his presentation “*Configurational Order-Disorder Transitions in ZnGeN₂*”. His presentation was cited for “highly-sophisticated solid state chemistry content, presented with clarity and perspective”.
- Dr. Max Wood, from the NASA Jet Propulsion Laboratory and Northwestern University, was recognized for his presentation “*The Effect of Multi-Band Transport on Thermal Conductivity Seen in Yb₁₄Mg_{1-x}Al_xSb₁₁*”. His work was cited as “exciting” and “impactful”, and his presentation “very nicely presents a new physical understanding encompassing detailed measurements and theory”.

Several speakers were further recognized with symposium awards (not disbursed from this grant):

- Xiucheng Wei, University of Buffalo, for his presentation “*Realization of BaZrS₃ Chalcogenide Perovskite Thin Films for Optoelectronics*”
- Jiang Chang-Ming, XXX, for his presentation “*Controlled Synthesis and Electronic Structure Engineering of Metastable Ta₂N₃ via Oxygen Incorporation*”
- Ida Sadeghi, University of Waterloo and Massachusetts Institute of Technology, for her presentation “*Late News: Growth of BaZrS₃ Thin Films by Molecular Beam Epitaxy*”

The panel discussion “*Why New Semiconductors?*” was lively and well-attended, and generated a lively debate among panelists on topics including compelling technology needs for semiconductors beyond silicon and III-Vs, important and outstanding fundamental questions in

semiconductor physics, and the professional hurdles facing research on new semiconductors. Below is a screenshot of the panel discussion including panelists and moderator:



4. ARO Support

ARO funds were used to support the conference registration of seven individuals whose participation was critical to the success of EL03.

2021 Virtual MRS Spring Meeting & Exhibit

Symposium SM12 : Bioinspired Macromolecular Assembly and Hybrid Materials—From Fundamental Science to Applications

Available on demand

2021-04-22

2021-04-23

2021-04-22 [+](#) Show All Abstracts

Symposium Organizers

Chun-Long Chen, Pacific Northwest National Laboratory
Fiona Meldrum, University of Leeds
Ki Tae Nam, Seoul National University
Tiffany Walsh, Deakin University

Symposium Support

Bronze
Army Research Office

Summary:

Symposium MS12 was held virtually at the 2021 MRS Spring Meeting and provided an international forum with a total of 16 invited speakers from Asian, North American, Europe to discuss the frontier research in the areas of bioinspired macromolecular assembly and hybrid materials. This symposium featured 41 oral presentations and 12 poster presentations. The symposium organizers presented eight best presentation awards.

Objectives:

Living organisms produce a wide variety of complex, nano-, micro-, and macroscale structured functional materials in an energy-efficient and highly reproducible manner, all under rather mild aqueous synthetic conditions. Throughout these processes, the specialized biomacromolecules, such as proteins and peptides, enables 1) hierarchical organization to assemble biomaterials and execute high-level functions; and 2) precise control over crystal nucleation, growth kinetics, phase transformation, and self-assembly, ultimately giving rise to biominerals with versatile functions. Inspired by nature, numerous approaches have been developed for the design and synthesis of bioinspired materials by using engineered proteins, peptides, DNAs, and other sequence-defined synthetic polymers (e.g. peptoids). These efforts address one of the grand challenges of materials science—to design and synthesize functional materials that rival those found in biology.

This symposium highlights recent developments in the areas of 1) bio-inspired macromolecular self-assembly to exploit (bio)macromolecules as building blocks to create hierarchical materials, and 2) biomimetic control over crystallization including a) bio-inspired control over inorganic (nano)crystal nucleation and growth, and b) nanoparticle self-assembly and attachment. This symposium will also address 3) the most recent insights obtained in the principles underlying (bio)macromolecular self-assembly and bio-controlled crystal formation (including using *in situ* molecular imaging and computational tools).

Research highlights:

The symposium presentations were divided into the following topic areas:

- 1) Bio-Inspired Hybrid Materials I, which includes three invited presentations. Prof. Takashi Kato from The University of Tokyo started this session by highlighting their recent development of nanorod and nanodisk hybrid materials based on calcium carbonate and hydroxyapatites. Prof. Shu Yang from University of Pennsylvania highlighted their recent development of bioinspired materials by self-assembly of polymeric colloidal particles. Prof. Nathaniel Rosi from University of Pittsburgh discussed their recent development of light-responsive shape-shifting nanoparticle superstructures.
- 2) Bio-Inspired Macromolecular Assembly, which includes a total of six presentations. Prof. Molly Stevens from Imperial College London started this session by highlighting her group's recent progress in the design of self-assembling materials for biomedical applications. Prof. Fabrizio Gelain from IRCCS Casa Sollievo della Sofferenza discussed their development of self-assembled peptide materials for regenerative medicine applications. Prof. Samuel Stupp concluded this session by highlighting their recent advances in the developing dynamic and bioactive peptide hydrogel materials as extracellular matrices for biomedical applications. Other speakers include Seungwook Ji and Han Kim from UC Berkeley and Ty Christoff-Tempesta from Massachusetts Institute of Technology.
- 3) Peptoid-based nanomaterials, which highlights six oral presentations in the self-assembly of peptoid nanomaterials. Prof. Galia Maayan from Technion–Israel Institute of Technology started this session by presenting the inclusion of metal-ligand coordination bonds in the peptoid design for the development of functional bio-inspired materials and supramolecular peptoid architectures. Prof. Adrienne Rosales from the University of Texas at Austin highlighted their recent development in exploiting sequence-defined peptoids as crosslinkers to build complexity and functionality into synthetic hydrogel biomaterials for tissue engineering applications. The third invited speaker in this session is Dr. Ronald Zuckermann from Lawrence Berkeley National Laboratory, who has invented the efficient, automated solid-phase peptoid synthesis. He pioneered the field of sequence control in biomimetic polymers and presented the development of peptoid-based nanomaterials and their characterizations of atomic structures. Other speakers include Madison Monahan, Jinrong Ma, and Shuai Zhang from University of Washington.
- 4) Bio-Inspired Hybrid Materials II, which includes three invited presentations and three contributed oral presentations. Prof. Marc Knecht from University of Miami started this session by highlighting their recent development of using peptide-based approaches to assemble graphene and hexagonal boron nitride (h-BN) nanosheets into three dimensions. A combination of experimental analyses and computational modeling was used to identify key parameters that control both the binding and the selectivity of peptides to these two materials. Prof. James De Yoreo from Pacific Northwest National Laboratory and University of Washington showed their recent studies of using in situ AFM to investigate the self-assembly of protein materials by using two types of engineered proteins and highlighted the importance of in situ imaging techniques in the mechanistic studies of macromolecular self-assembly. Prof. David Kisailus from University of California Irvine highlighted their recent studies of the tooth formation of *Cryptochiton stelleri* found in the eastern Pacific and their bioinspired materials synthesis inspired by such biomineralization studies. Other speakers include Susrut Akkineni from University of Washington, Kenan Song from Arizona State University, Tyler Jorgenson from University of Washington.

- 5) Bio-Inspired Hybrid Materials III and Poster Session. This session started with Dr. Shunzhi Wang's presentation by highlighting his research did at the Northwestern University of using DNA as a particle-directing ligand to control colloidal crystal assembly. Followed by two oral presentations: one from Junhua Yu from Seoul National University and another from Muammer Yaman from University of Washington, we had nice 5-min flash talks for the poster sessions. For example, Tong Li from University of Wisconsin-Madison discussed about their recent discovery of using self-assembled poly-L-lactic acid/Glycine nanofibers for high piezoelectricity. Kathryn Guye from University of Washington discussed their recent study of using surface charges of protein fibers to influence the assembly of metal nanoparticles. Amy Stegmann from University of Washington presented their study of using de novo protein templates for controlling TiO₂ mineralization.
- 6) Bio-Inspired Macromolecular Self-Assembly. Prof. Jing Sun from Qingdao University of Science and Technology started this session by having an invited talk to highlight her group's recent development of self-assembly of polypeptoids into various nanostructures including 2D crystalline nanosheets and superbrushes. Runye Zha from Rensselaer Polytechnic Institute discussed their recent development of using self-assembly of silk fibroin and silk-like macromolecules for biomimetic coatings. Zijie Wu from University of Delaware presented their recent development of a coarse-grained (CG) model to simulate the assembly of cellulose and cellulose derivatives (e.g. methylcellulose).
- 7) Bio-Inspired Macromolecular Assembly. This is a joint session with symposium 09 co-chaired by Prof. Chis Kloxin and Dr. Chun-Long Chen. This session includes three invited presentations which Prof. Pochan Darrin started this session by highlighting their recent development in exploiting peptide "bundlemer" to assemble bioinspired nanomaterials. Other two invited speakers are Prof. David Baker from University of Washington and Prof. Akif Tezcan from University of California, San Diego. Prof. Baker discussed their recent progress in exploring the de novo design of proteins for the self-assembly of 1D nanofibers, 2D network and 3D crystal architectures. He further highlighted their progress in the design and assembly of protein-inorganic hybrid materials. Prof. Tezcan discussed their recent progress in design and self-assembly of proteins into various dynamic and adaptive materials by using strategies based on metal-ligand coordination and polymer chemistry.
- 8) Bio-Inspired Hybrid Materials IV. This session contains six contributed oral presentations. Arash Momeni started this session by showing their recent development of polymeric fibers based on cellulose nanocrystals (CNCs). Prof. Jinlian Hu from presented her group recently progress in the self-assembly of spiker silk fiber materials and their applications including directional water collection.

Contributions to the Discipline:

This symposium (**SM12**) brought together an interdisciplinary group of scientists and engineers from all over the world, including materials scientists, chemists, physicists, theorists to understand the bio-inspired macromolecular self-assembly and biomimetic crystallization for developing functional materials for applications. This symposium helped students and postdocs to learn the recent progress in the development of bioinspired nanomaterials and materials characterizations. This symposium offered a forum for scientists from multidisciplinary fields to exchange new ideas and potentially create new directions in bio-inspired materials synthesis. The organizers believe that the ideas and

collaborations from this symposium SM12 will make significant impacts in the design and synthesis of new functional materials and bring bioinspired research to a new high level in the near future.

Symposium SM12 organizer used the ARO grant (\$2500) to pay for partial registration fees for 10 invited speakers and two co-organizers ($\$150 \times 12 = \1800), and seven selected excellent presentations from students and postdocs ($\$100 \times 7 = \700).

Supported Invited Speakers (or Co-Organizers)

Marc Knecht, University of Miami

Galia Maayan, Technion - Israel Institute of Technology

Adrienne Rosales, The University of Texas at Austin

Nathaniel Rosi, University of Pittsburgh

Molly Stevens, Imperial College London

Samuel Stupp, Northwestern University

Ki Tae Nam, Seoul National University

Fiona Meldrum, University of Leeds

James J. De Yoreo, Pacific Northwest National Laboratory

Fabrizio Gelain, Fondazione Istituto di Ricovero e Cura a Carattere Scientifico Casa Sollievo della Sofferenza

Takashi Kato, The University of Tokyo

David Kisailus, University of California, Irvine

Excellent symposium presentation awards

Han Kim, University of California, Berkeley

Ty Christoff-Tempesta, MIT

Madison Monahan, University of Washington

Susrut Akkineni, University of Washington

Shunzhi Wang, Northwestern University

Zijie Wu, University of Delaware

Evan Mueller, University of Colorado Boulder

Future Directions:

Energy sustainability, human health, and security remain a critical issue of our society, for which bioinspired synthesis of functional materials will play an important role. MRS has long recognized this fact and embraced the challenge in every meeting, and this trend is expected to continue at a

higher level of momentum in the foreseeable future. The integration of bioinspired materials synthesis, advanced characterization techniques, and computational simulations is expected to promote research efforts in this field. Further conference symposia of this theme will serve to accelerate our efforts.

Acknowledgements:

The organizers gratefully appreciate the support from the US Army Research Office (ARO), which was critical to the success of this symposium. We also want to thank MRS staff for supporting the application of this ARO grant.